

Algorithms for reasoning with graphical models

Class 1
Rina Dechter

Dechter-Morgan&claypool book (Dbook): Chapters 1-2

Outline

- **Graphical models:** The constraint network, Probabilistic networks, cost networks and mixed networks. queries: consistency, counting, optimization and likelihood queries.
- **Inference: Bucket elimination for deterministic networks** (Adaptive-consistency, and the Davis-Putnam algorithms.) The induced-width
 - **Inference: Bucket-elimination for Bayesian and Markov networks** queries (mpe, map, marginal and probability of evidence)
 - **Graph properties:** induced-width, tree-width, chordal graphs, hypertrees, join-trees.
 - **Inference: Tree-decomposition algorithms** (join-tree propagation and junction-trees)
- **Approximation by bounded Inference:** (weighted Mini-bucket , belief/constraint-propagation, constraint propagation, generalized belief propagation, variational methods)
- **Search for csps: Backtracking;** pruning search by constraint propagation, backjumping and learning.
- **Search: AND/OR search Spaces** for likelihood, optimization queries (Probability of evidence, Partition function, MAP and MPE queries, AND/OR branch and bound).
- **Approximation by sampling:** Gibbs sampling, Importance sampling, cutset-sampling, SampleSearch and AND/OR sampling, Stochastic Local Search.
- **Hybrid of search Inference:** cutset-conditioning and cutset-sampling

Outline

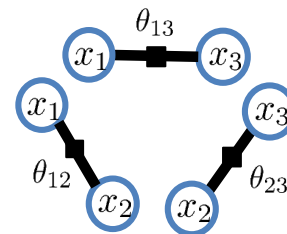
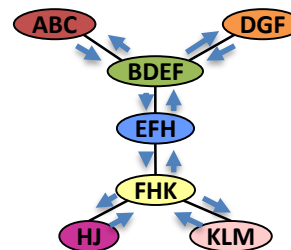
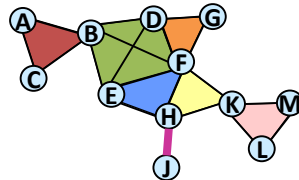
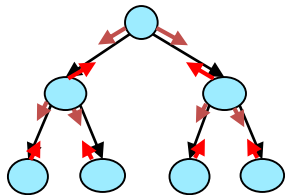
- **Graphical models:** The constraint network, Probabilistic networks, cost networks and mixed networks. Graphical representations and queries: consistency, counting, optimization and likelihood queries.
- **Constraints inference: Bucket elimination** for deterministic networks (Adaptive-consistency, and the Davis-Putnam algorithms.) The induced-width.
- Inference: Bucket-elimination for Bayesian and Markov networks queries (mpe, map, marginal and probability of evidence)
- Graph properties: induced-width, tree-width, chordal graphs, hypertrees, join-trees.
- Inference: Tree-decomposition algorithms (join-tree propagation and junction-trees algorithm, Cluster tree-elimination.)
- Approximation by bounded Inference: (Mini-bucket , belief-propagation, constraint propagation, generalized belief propagation)
- Search: Backtracking search algorithms; pruning search by constraint propagation, backjumping and learning.

Course Requirements/Textbook

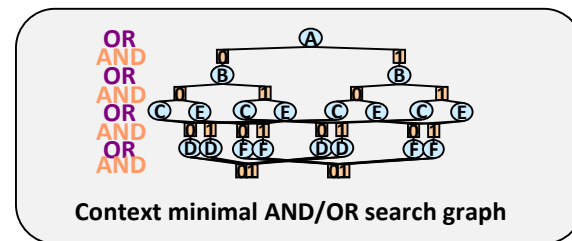
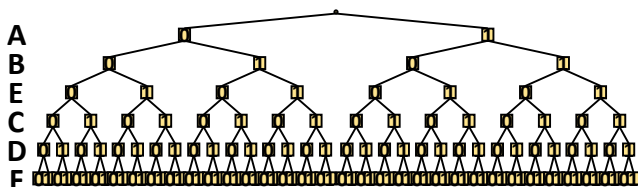
- Homeworks : There will be 5-6 problem sets , graded 70% of the final grades.
- A term project: paper presentation, a programming project.
- Books:
 - “Reasoning with probabilistic and deterministic graphical models”, R. Dechter, Claypool, 2013
<https://www.morganclaypool.com/doi/abs/10.2200/S00529ED1V01Y201308AIM023>
 - “Modeling and Reasoning with Bayesian Networks”, A. Darwiche, MIT Press, 2009.
 - “Constraint Processing” , R. Dechter, Morgan Kauffman, 2003

Outline of classes

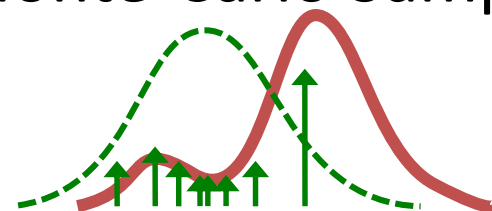
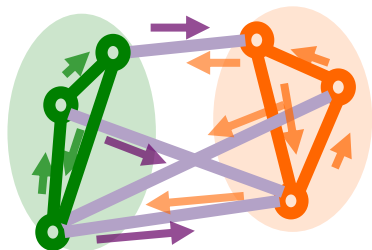
- Part 1: Introduction and Inference



- Part 2: Search

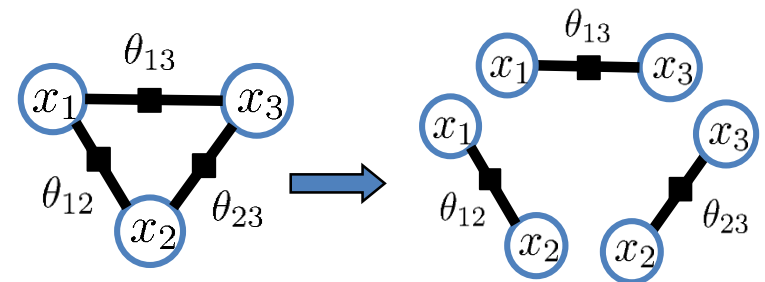
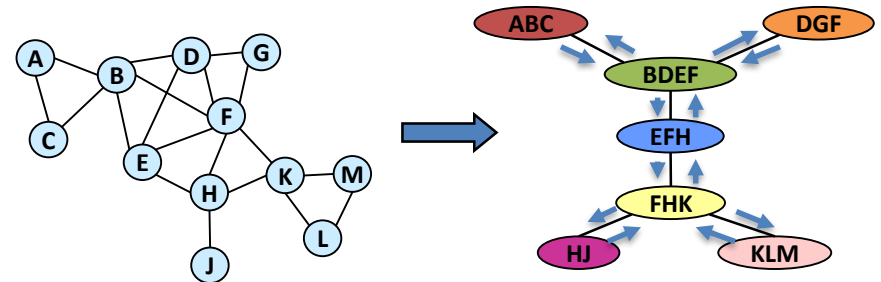
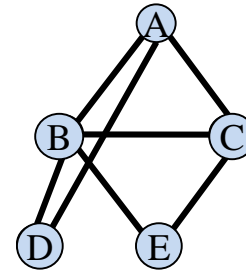


- Part 3: Variational Methods and Monte-Carlo Sampling



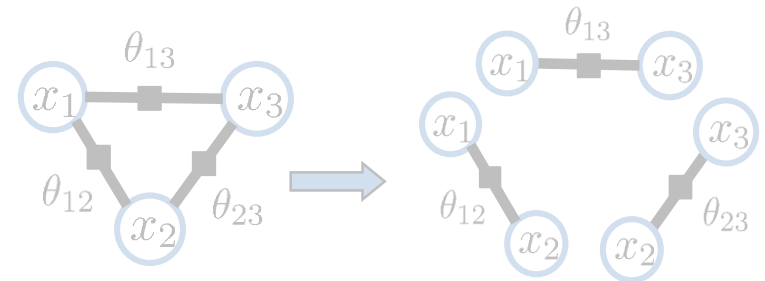
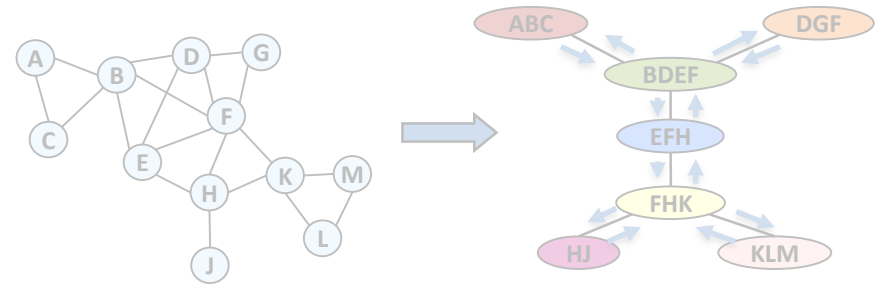
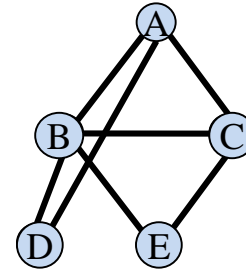
RoadMap: Introduction and Inference

- Basics of graphical models
 - Queries
 - Examples, applications, and tasks
 - Algorithms overview
- Inference algorithms, exact
 - Bucket elimination for trees
 - Bucket elimination
 - Jointree clustering
 - Elimination orders
- Approximate elimination
 - Decomposition bounds
 - Mini-bucket & weighted mini-bucket
 - Belief propagation
- Summary and Part 2



RoadMap: Introduction and Inference

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Probabilistic Graphical models

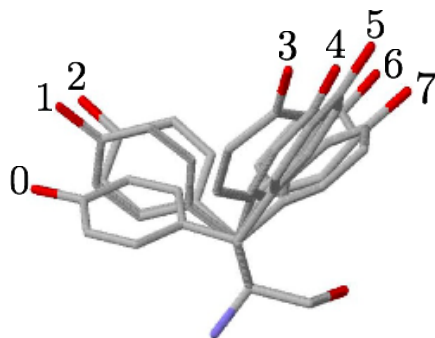
- Describe structure in large problems
 - Large complex system $F(X)$
 - Made of “smaller”, “local” interactions $f_\alpha(x_\alpha)$
 - Complexity emerges through interdependence

Probabilistic Graphical models

- Describe structure in large problems
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 - Complexity emerges through interdependence
- Examples & Tasks
 - Maximization (MAP): compute the most probable configuration

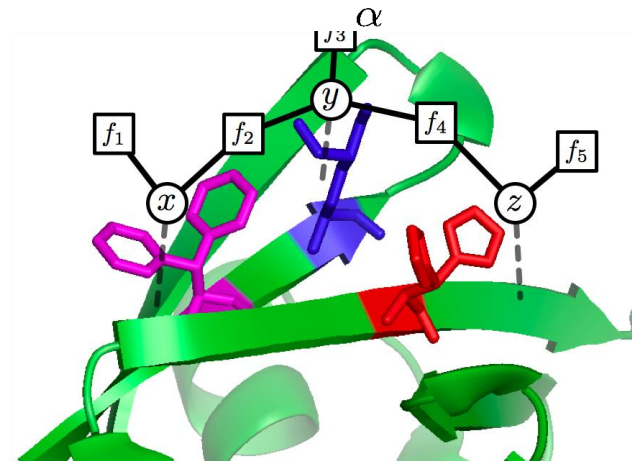
$$\mathbf{x}^* = \arg \max_{\mathbf{x}} \prod_{\alpha} f_{\alpha}(\mathbf{x}_{\alpha})$$

$$f(\mathbf{x}^*) = \max_{\mathbf{x}} \prod_{\alpha} f_{\alpha}(\mathbf{x}_{\alpha})$$



Phenylalanine

[Yanover & Weiss 2002]



Probabilistic Graphical models

- Describe structure in large problems
 - Large complex system $F(X)$
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- Examples & Tasks

- Summation & marginalization

$$p(x_i) = \frac{1}{Z} \sum_{\mathbf{x} \setminus x_i} \prod_{\alpha} f_{\alpha}(\mathbf{x}_{\alpha}) \quad \text{and}$$

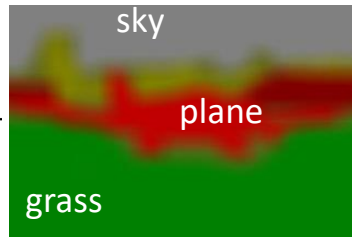
“partition function”

$$Z = \sum_{\mathbf{x}} \prod_{\alpha} f_{\alpha}(\mathbf{x}_{\alpha})$$

Observation \mathbf{y}



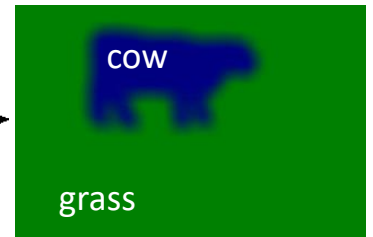
Marginals $p(x_i | \mathbf{y})$



Observation \mathbf{y}



Marginals $p(x_i | \mathbf{y})$



e.g., [Plath et al. 2009]

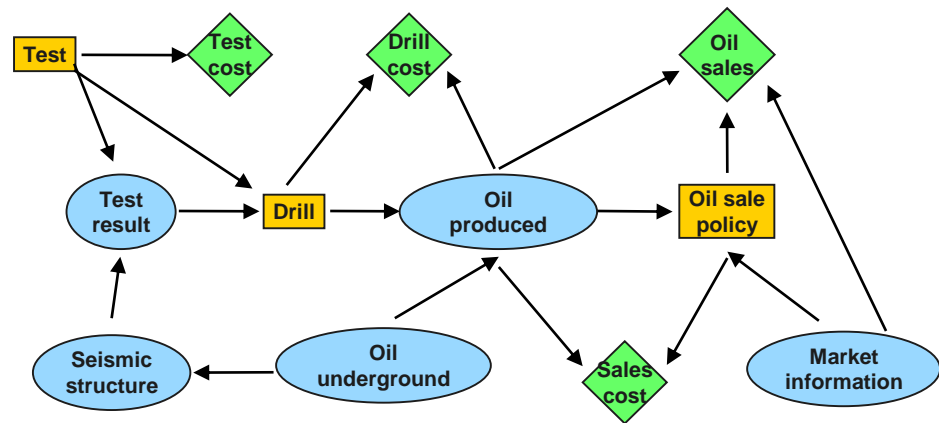
Graphical models

- Describe structure in large problems
 - Large complex system $F(X)$
 - Made of “smaller”, “local” interactions $f_\alpha(x_\alpha)$
 - Complexity emerges through interdependence
- Examples & Tasks
 - Mixed inference (marginal MAP, MEU, ...)

$$f(\mathbf{x}_M^*) = \max_{\mathbf{x}_M} \sum_{\mathbf{x}_S} \prod_{\alpha} f_{\alpha}(\mathbf{x}_{\alpha})$$

Influence diagrams &
optimal decision-making

(the “oil wildcatter” problem)



e.g., [Raiffa 1968; Shachter 1986]

In more details...

Constraint Networks

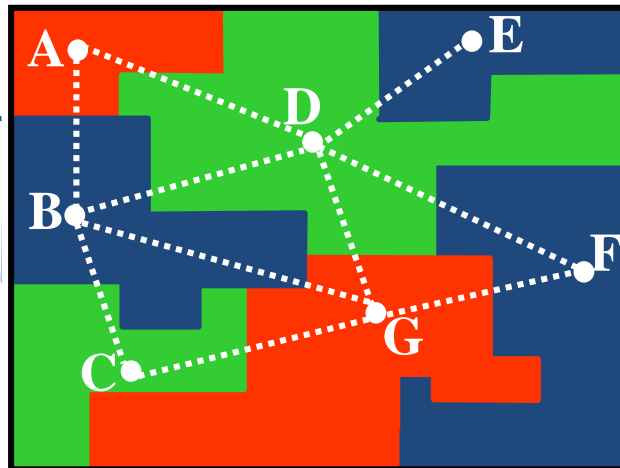
Example: map coloring

Variables - countries (A,B,C,etc.)

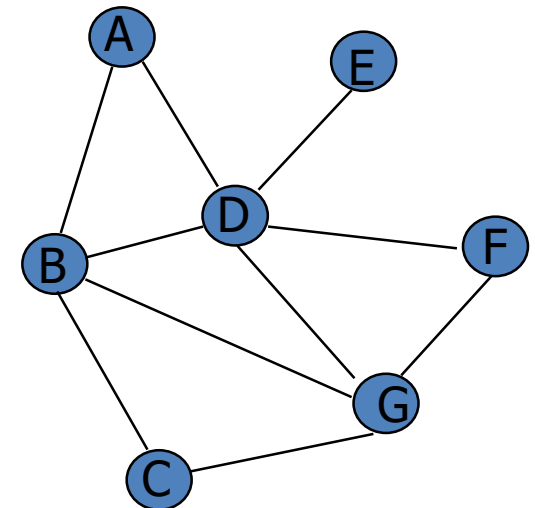
Values - colors (red, green, blue)

Constraints: **$A \neq B$** , $A \neq D$, $D \neq E$, etc.

A	B
red	green
red	yellow
green	red
green	yellow
yellow	green
yellow	red



Constraint graph



Propositional Reasoning

Example: party problem

- If Alex goes, then Becky goes:
- If Chris goes, then Alex goes:

$$A \rightarrow B$$

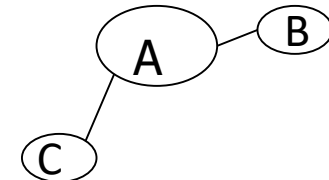
$$C \rightarrow A$$

- **Question:**

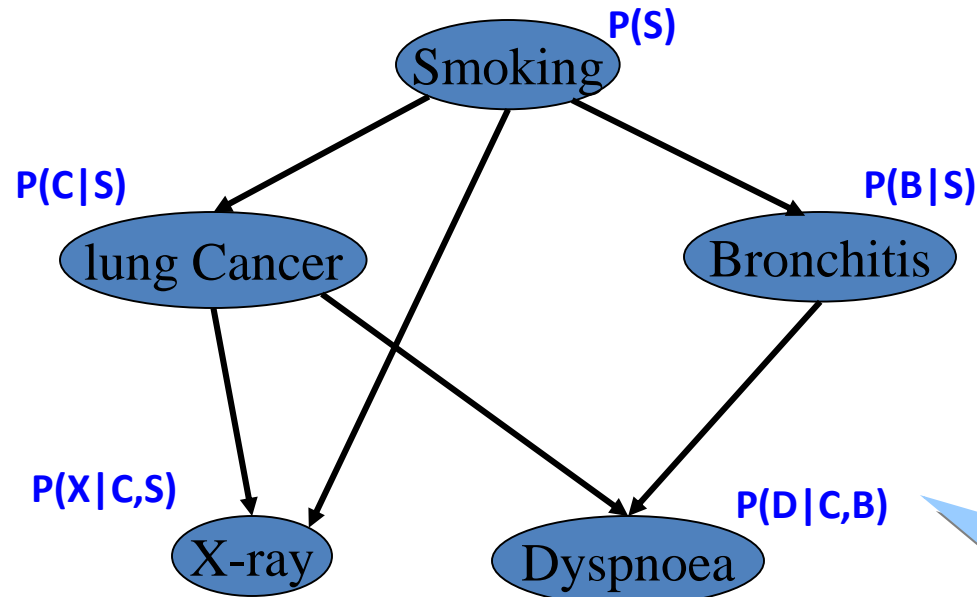
Is it possible that Chris goes to the party but Becky does not?

Is the *propositional theory*

$\varphi = \{A \rightarrow B, C \rightarrow A, \neg \mathbf{B}, \mathbf{C}\}$ satisfiable?



Bayesian Networks (Pearl 1988)



$$\mathbf{BN} = (\mathbf{G}, \Theta)$$

CPD:

C	B	$P(D C,B)$	
0	0	0.1	0.9
0	1	0.7	0.3
1	0	0.8	0.2
1	1	0.9	0.1

$$P(S, C, B, X, D) = P(S) P(C|S) P(B|S) P(X|C,S) P(D|C,B)$$

Combination: Product
Marginalization: sum/max

- Posterior marginals, probability of evidence, MPE

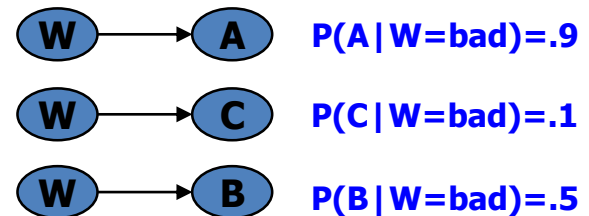
$$P(D=0) = \sum_{S,L,B,X} P(S) \cdot P(C|S) \cdot P(B|S) \cdot P(X|C,S) \cdot P(D|C,B)$$

$$\text{MAP}(P) = \max_{S,L,B,X} P(S) \cdot P(C|S) \cdot P(B|S) \cdot P(X|C,S) \cdot P(D|C,B)$$

Probabilistic reasoning (directed)

Party example: the weather effect

- Alex is likely-to-go in bad weather
- Chris rarely-goes in bad weather
- Becky is indifferent but unpredictable



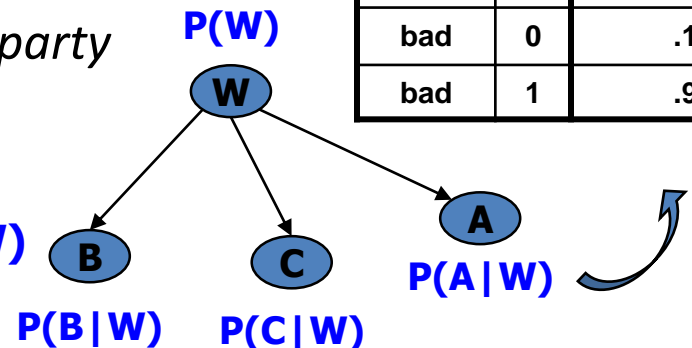
Questions:

- Given bad weather, which group of individuals is most likely to show up at the party?
- What is the probability that Chris goes to the party but Becky does not?

W	A	$P(A W)$
good	0	.01
good	1	.99
bad	0	.1
bad	1	.9

$$P(W, A, C, B) = P(B | W) \cdot P(C | W) \cdot P(A | W) \cdot P(W)$$

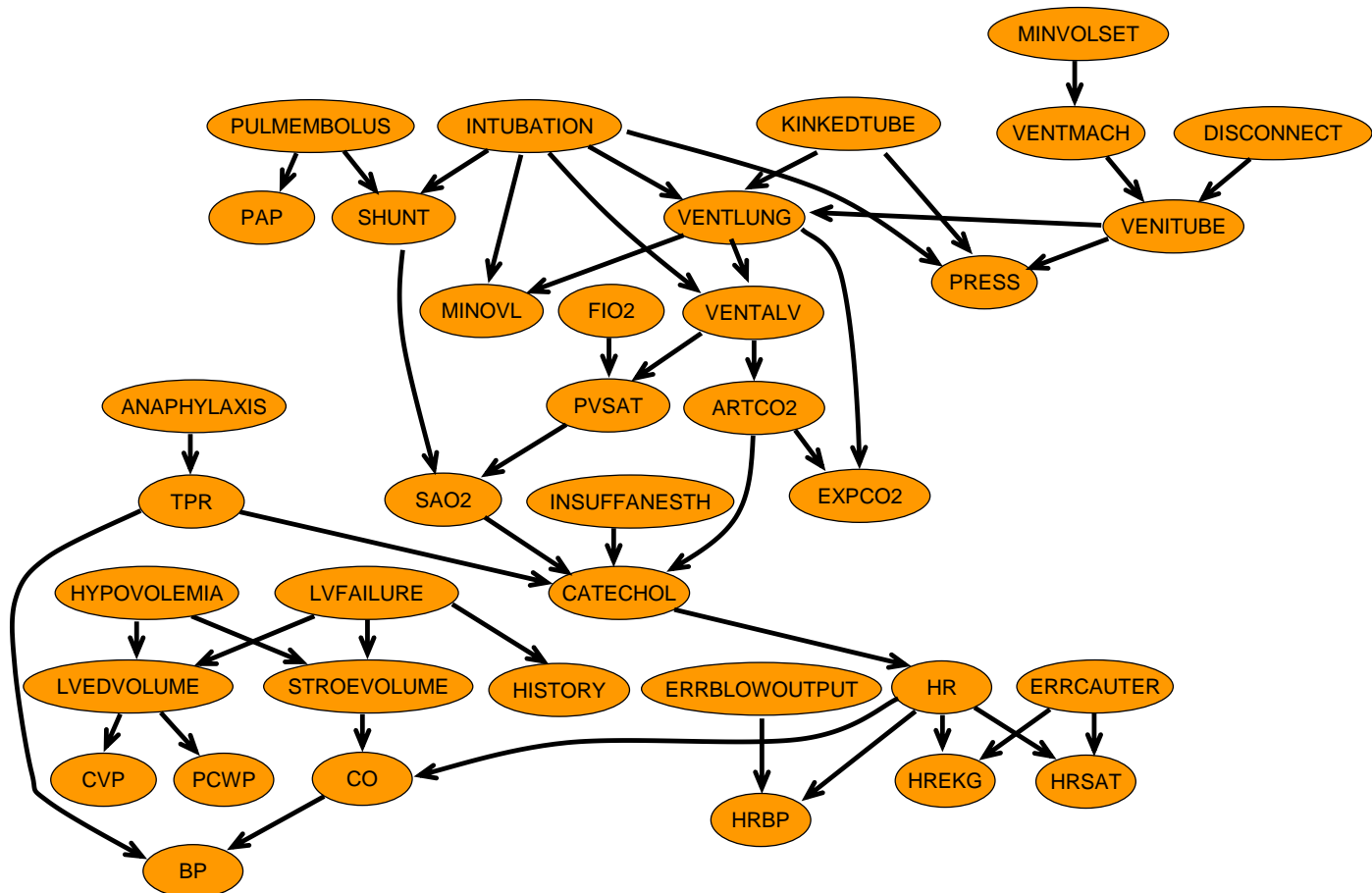
$$P(A, C, B | W=\text{bad}) = 0.9 \cdot 0.1 \cdot 0.5$$



Alarm network [Beinlich et al., 1989]

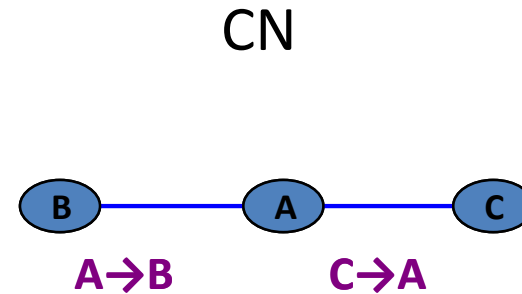
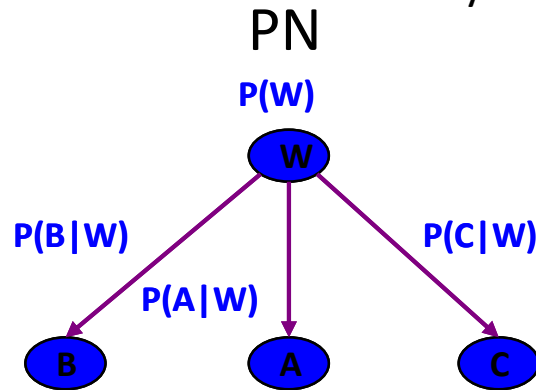
- Bayes nets: compact representation of large joint distributions

The “alarm” network: 37 variables, 509 parameters (rather than $2^{37} = 10^{11}$!)



Mixed Probabilistic and Deterministic networks

Alex is likely-to-go in bad weather
Chris rarely-goes in bad weather
Becky is indifferent but unpredictable



Query:

Is it likely that Chris goes to the party if Becky does not but the weather is bad?

$$P(C, \neg B \mid w = \text{bad}, A \rightarrow B, C \rightarrow A)$$

Graphical models (cost networks)

Example:

A *graphical model* consists of:

$X = \{X_1, \dots, X_n\}$ -- variables

$D = \{D_1, \dots, D_n\}$ -- domains (we'll assume discrete)

$F = \{f_{\alpha_1}, \dots, f_{\alpha_m}\}$ -- functions or “factors”

and a *combination operator*

$$A \in \{0, 1\}$$

$$B \in \{0, 1\}$$

$$C \in \{0, 1\}$$

$$f_{AB}(A, B), \quad f_{BC}(B, C)$$

The *combination operator* defines an overall function from the individual factors,

e.g., “+” : $F(A, B, C) = f_{AB}(A, B) + f_{BC}(B, C)$

Notation:

Discrete X_i values called **states**

Tuple or **configuration**: states taken by a set of variables

Scope of f : set of variables that are arguments to a factor f

often index factors by their scope, e.g., $f_{\alpha}(X_{\alpha})$, $X_{\alpha} \subseteq X$

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$$C \in \{0, 1\}$$

$$f_{AB}(A, B), \quad f_{BC}(B, C)$$

For discrete variables, think of functions as “tables”
(though we might represent them more efficiently)

A	B	f(A,B)
0	0	6
0	1	0
1	0	0
1	1	6

+

B	C	f(B,C)
0	0	6
0	1	0
1	0	0
1	1	6

=

$$F(A = 0, B = 1, C = 1)$$

A	B	C	f(A,B,C)
0	0	0	12
0	0	1	6
0	1	0	0
0	1	1	6
1	0	0	6
1	0	1	0
1	1	0	6
1	1	1	12

$$= 0 + 6$$

Graph Visualiization: Primal Graph

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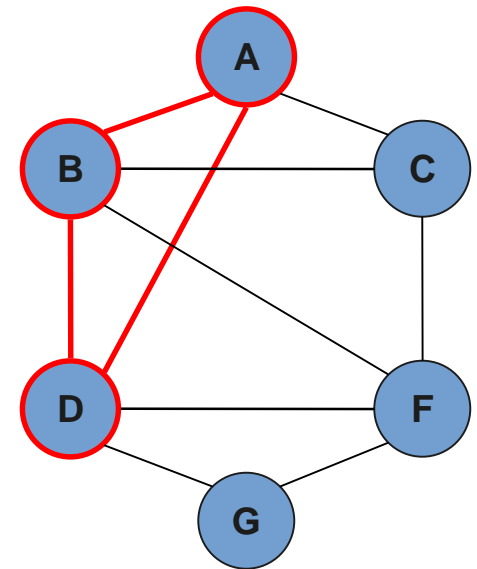
and a *combination operator*

Primal graph:

variables \rightarrow nodes

factors \rightarrow cliques

$$F(A, B, C, D, F, G) = f_1(A, B, D) + f_2(D, F, G) \\ + f_3(B, C, F) + f_4(A, C)$$



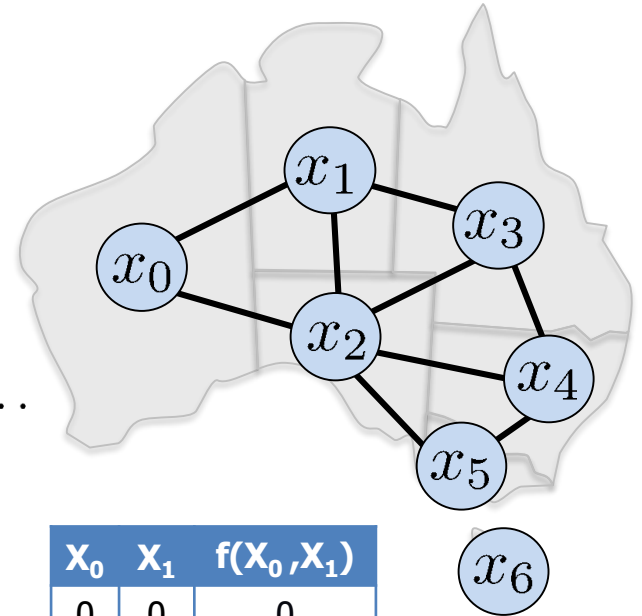
Example: Constraint networks

$$X_i \in \{\text{red}, \text{green}, \text{blue}\}$$

$$f_{ij}(X_i, X_j) = (X_i \neq X_j) \quad \text{for adjacent regions } i, j$$

Overall function is “and” of individual constraints:

$$F(X) = f_{01}(X_0, X_1) \wedge f_{12}(X_1, X_2) \wedge f_{02}(X_0, X_2) \wedge \dots$$



“Tabular” form:

$$f_{ij}(X_i, X_j) = \begin{cases} 1.0 & X_i \neq X_j \\ 0.0 & X_i = X_j \end{cases}$$

$$F(X) = \prod_{ij} f_{ij}(X_i, X_j) = \begin{cases} 1.0 & \text{all valid} \\ 0.0 & \text{any invalid} \end{cases}$$

Tasks: “max”: is there a solution?

“sum”: how many solutions?

x_0	x_1	$f(x_0, x_1)$
0	0	0
0	1	1
0	2	1
1	0	1
1	1	0
1	2	1
2	0	1
2	1	1
2	2	0

Markov logic, Markov networks

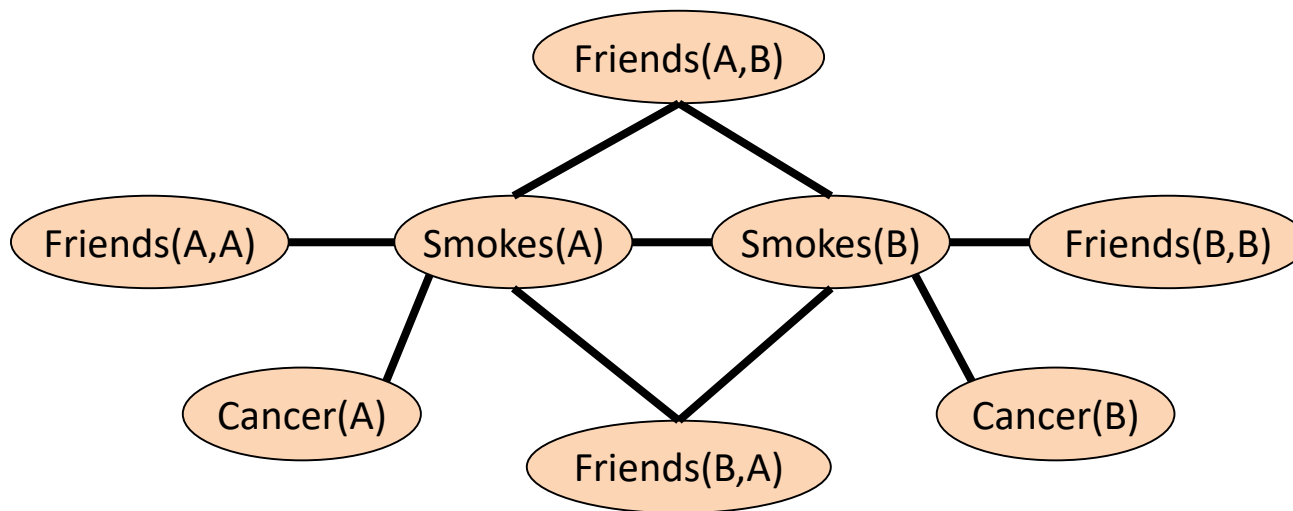
[Richardson & Domingos 2005]

1.5 $\forall x \text{ Smokes}(x) \Rightarrow \text{Cancer}(x)$

1.1 $\forall x, y \text{ Friends}(x, y) \Rightarrow (\text{Smokes}(x) \Leftrightarrow \text{Smokes}(y))$

Two constants: **Anna** (A) and **Bob** (B)

S_A	C_A	$f(S_A, C_A)$
0	0	$\exp(1.5)$
0	1	$\exp(1.5)$
1	0	1.0
1	1	$\exp(1.5)$



F_{AB}	S_A	S_B	$f(\cdot)$
0	0	0	$\exp(1.1)$
0	0	1	$\exp(1.1)$
0	1	0	$\exp(1.1)$
0	1	1	$\exp(1.1)$
1	0	0	$\exp(1.1)$
1	0	1	1.0
1	1	0	1.0
1	1	1	$\exp(1.1)$

Graphical visualization

A *graphical model* consists of:

$X = \{X_1, \dots, X_n\}$ -- variables

$D = \{D_1, \dots, D_n\}$ -- domains

$F = \{f_{\alpha_1}, \dots, f_{\alpha_m}\}$ -- functions or “factors”

and a *combination operator*

Primal graph:

variables \rightarrow nodes

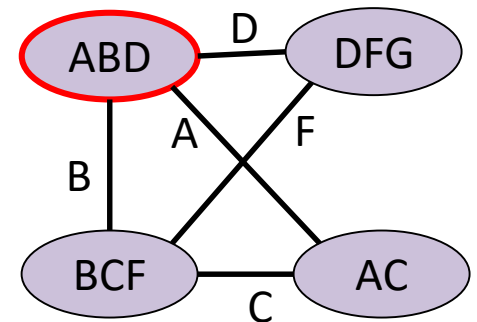
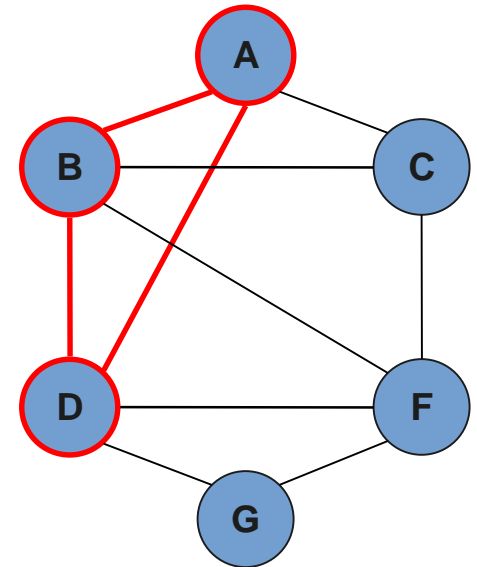
factors \rightarrow cliques

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Dual graph:

factor scopes \rightarrow nodes

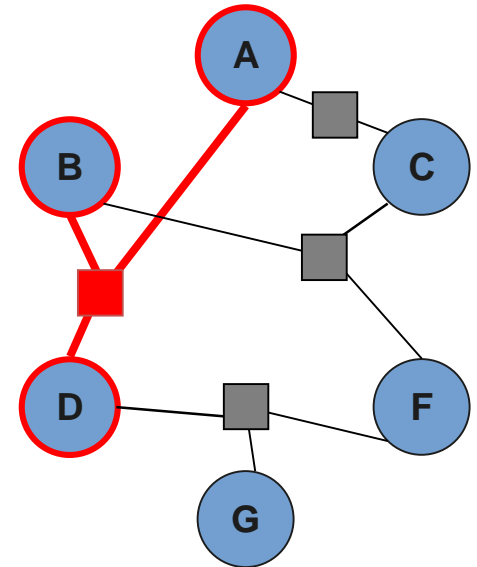
edges \rightarrow intersections (separators)



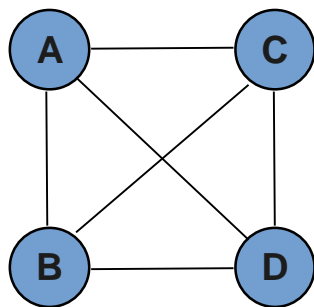
Graphical visualization

“Factor” graph: explicitly indicate the scope of each factor
 variables \rightarrow circles
 factors \rightarrow squares

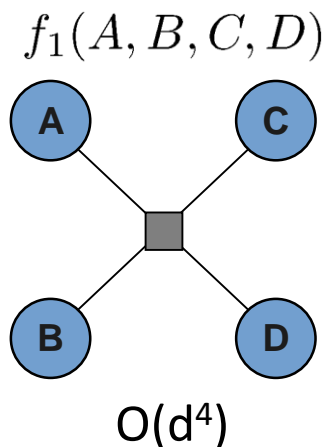
$$F(A, B, C, D, F, G) = f_1(A, B, D) + f_2(D, F, G) + f_3(B, C, F) + f_4(A, C)$$



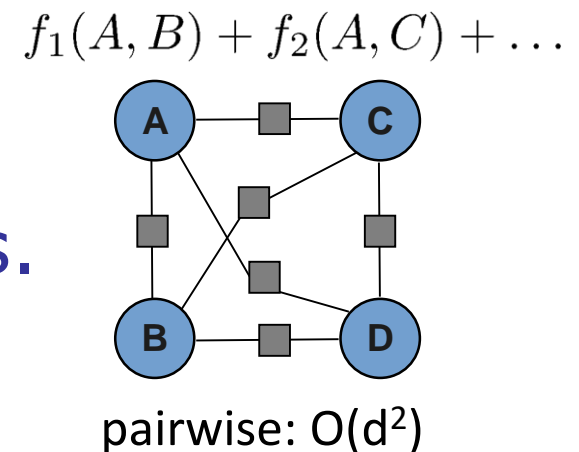
Useful for disambiguating factorization:



$\stackrel{?}{=}$



vs.



Graphical models

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$F = \{f_{\alpha_1}, \dots, f_{\alpha_m}\}$ -- functions or “factors”

Operators:

combination operator
(sum, product, join, ...)

elimination operator
(projection, sum, max, min, ...)

Types of queries:

Marginal: $Z = \sum_{\mathbf{x}} \prod_{\alpha} f_{\alpha}(\mathbf{x}_{\alpha})$

MPE / MAP: $f(\mathbf{x}^*) = \max_{\mathbf{x}} \prod_{\alpha} f_{\alpha}(\mathbf{x}_{\alpha})$

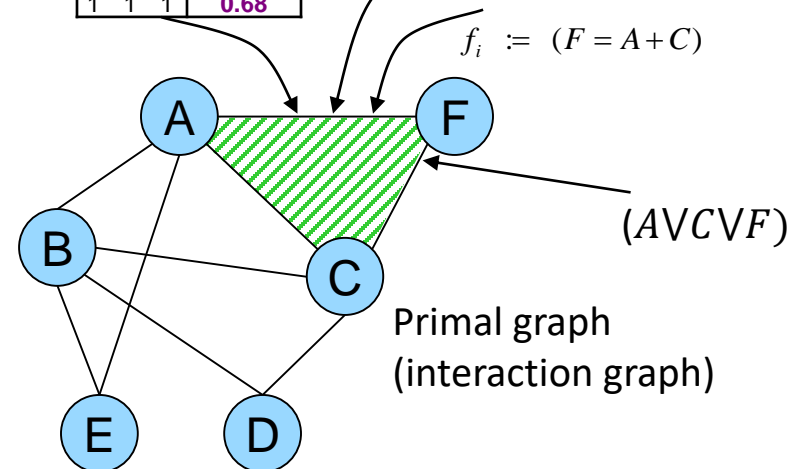
Marginal MAP: $f(\mathbf{x}_M^*) = \max_{\mathbf{x}_M} \sum_{\mathbf{x}_S} \prod_{\alpha} f_{\alpha}(\mathbf{x}_{\alpha})$

Conditional Probability
Table (CPT)

A	C	F	P(F A,C)
0	0	0	0.14
0	0	1	0.96
0	1	0	0.40
0	1	1	0.60
1	0	0	0.35
1	0	1	0.65
1	1	0	0.72
1	1	1	0.68

Relation

A	C	F
red	green	blue
blue	red	red
blue	blue	green
green	red	blue



- All these tasks are NP-hard
 - exploit problem structure
 - identify special cases
 - approximate

Graphical models/reasoning task

Definition 2.1.2 (graphical model) A graphical model \mathcal{M} is a 4-tuple, $\mathcal{M} = \langle \mathbf{X}, \mathbf{D}, \mathbf{F}, \otimes \rangle$, where:

1. $\mathbf{X} = \{X_1, \dots, X_n\}$ is a finite set of variables;
2. $\mathbf{D} = \{D_1, \dots, D_n\}$ is the set of their respective finite domains of values;
3. $\mathbf{F} = \{f_1, \dots, f_r\}$ is a set of positive real-valued discrete functions, defined scopes of variables $S_i \subseteq \mathbf{X}$,
4. \otimes is a combination operator¹ (e.g., $\otimes \in \{\prod, \sum, \bowtie\}$ (product, sum, join)).

The graphical model represents a global function whose scope is \mathbf{X} which is the combination of all its functions: $\otimes_{i=1}^r f_i$.

Definition 2.1.3 (a reasoning problem) A reasoning problem over a graphical model $\mathcal{M} = \langle \mathbf{X}, \mathbf{D}, \mathbf{F}, \otimes \rangle$ and a subset of variable $Y \subset \mathbf{X}$ is defined by a marginalization operator \Downarrow_Y . If S is the scope of function f then $\Downarrow_Y f \in \{\max_{S-Y} f, \min_{S-Y} f, \pi_Y f, \sum_{S-Y} f\}$ is a marginalization operator. The reasoning problem $\mathcal{P}\langle \mathcal{M}, \Downarrow_Y, \mathbf{Z} \rangle$ is the task of computing the function $\mathcal{P}_{\mathcal{M}}(\mathbf{Z}) = \Downarrow_{\mathbf{Z}} \otimes_{i=1}^r f_i$, where r is the number of functions in \mathbf{F} .

Summary of graphical models types

- Constraint networks
- Cost networks
- Bayesian network
- Markov networks
- Mixed probability and constraint network
- Influence diagrams

Constraint Networks

Map coloring

Variables: countries (A B C etc.)

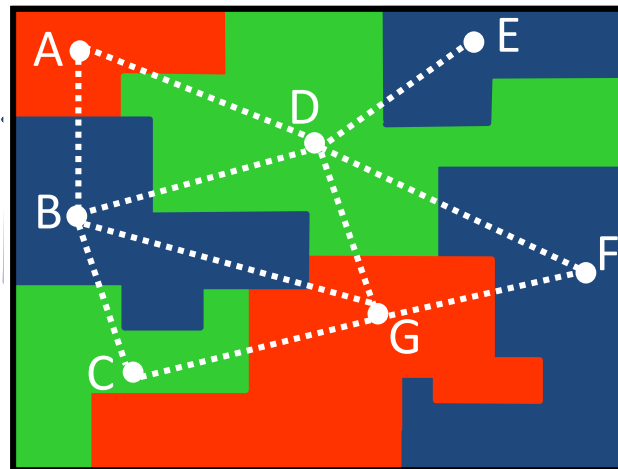
Values: colors (red green blue)

Constraints: **A \neq B, A \neq D, D \neq E, ...**

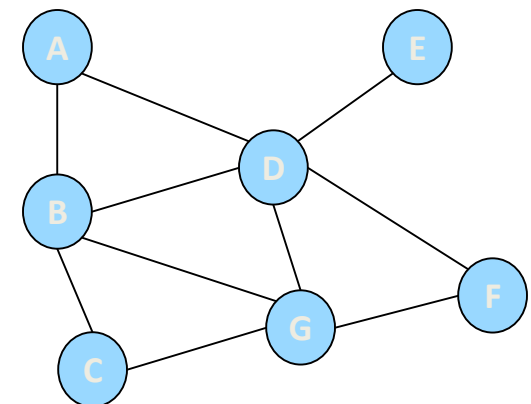
Combination = join

Marginalization = projection

A	B
red	green
red	yellow
green	red
green	yellow
yellow	green
yellow	red



Constraint graph



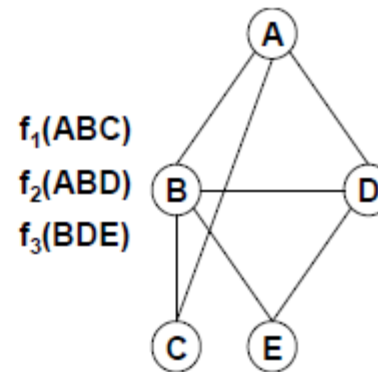
Example of a Cost Network

A	B	C	$f_1(ABC)$
0	0	0	∞
0	0	1	∞
0	1	0	∞
0	1	1	2
1	0	0	∞
1	0	1	2
1	1	0	∞
1	1	1	2

A	B	D	$f_2(ABD)$
0	0	0	1
0	0	1	∞
0	1	0	0
0	1	1	2
1	0	0	6
1	0	1	5
1	1	0	6
1	1	1	5

B	D	E	$f_3(BDE)$
0	0	0	∞
0	0	1	3
0	1	0	∞
0	1	1	4
1	0	0	∞
1	0	1	3
1	1	0	∞
1	1	1	4

(a) Cost functions



(b) Constraint graph

Figure 2.3: A cost network.

Combination: sum

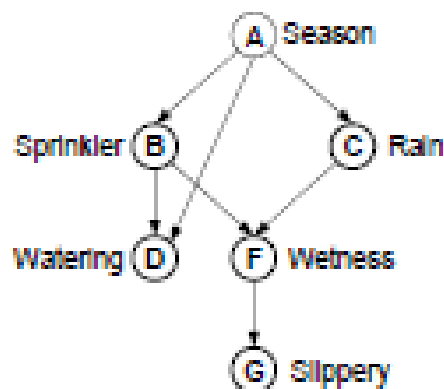
Marginalization: min/max

Definition 2.3.2 (WCSP) A Weighted Constraint Satisfaction Problem (WCSP) is a graphical model $\langle X, D, F, \sum \rangle$ where each of the functions $f_i \in F$ assigns "0" (no penalty) to allowed tuples and a positive integer penalty cost to the forbidden tuples. Namely, $f_i : D_{X_{i_1}} \times \dots \times D_{X_{i_t}} \rightarrow \mathbb{N}$, where $S_i = \{X_{i_1}, \dots, X_{i_t}\}$ is the scope of the function.

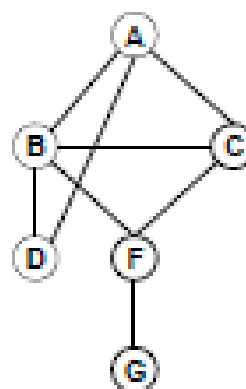
A Bayesian Network

B	C	F	$P(F B, C)$	B	$A = \text{winter}$	D	$P(D A, B)$
false	false	true	0.1	false	false	true	0.3
true	false	true	0.9	true	false	true	0.9
false	true	true	0.8	false	true	true	0.1
true	true	true	0.95	true	true	true	1

A	C	$P(C A)$	A	B	$P(B A)$	F	G	$P(G F)$
Summer	true	0.1	Summer	true	0.8	false	true	0.1
Fall	true	0.4	Fall	true	0.4	true	true	1
Winter	true	0.9	Winter	true	0.1			
Spring	true	0.3	Spring	true	0.6			



(a) Directed acyclic graph

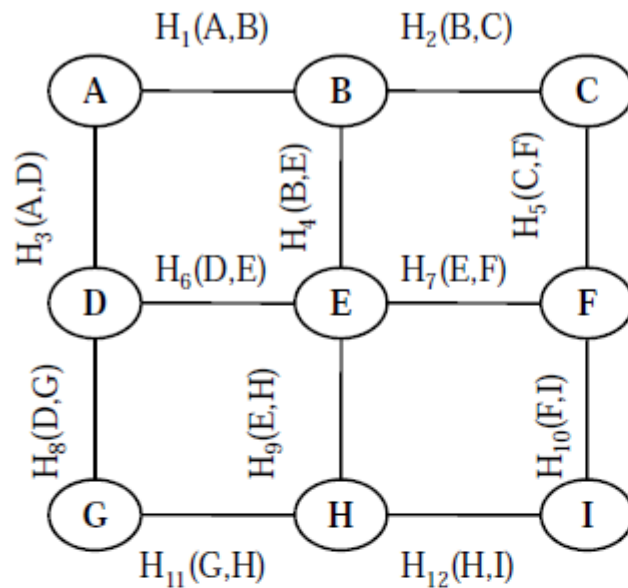


(b) Moral graph

Combination: product
Marginalization: sum or min/max

Belief network $P(g, f, c, b, a) = P(g|f)P(f|c, b)P(d|a, b)P(c|1)P(b|a)P(a)$

Markov Networks



(a)

D	E	$H_6(D,E)$
0	0	20.2
0	1	12
1	0	23.4
1	1	11.7

(b)

Figure 2.6: (a) An example 3×3 square Grid Markov network (ising model) and (b) An example potential $H_6(D, E)$

network represents a global joint distribution over the variables \mathbf{X} given by:

$$P(\mathbf{x}) = \frac{1}{Z} \prod_{i=1}^m H_i(\mathbf{x}) \quad , \quad Z = \sum_{\mathbf{x} \in \mathbf{X}} \prod_{i=1}^m H_i(\mathbf{x})$$

Example domains for graphical models

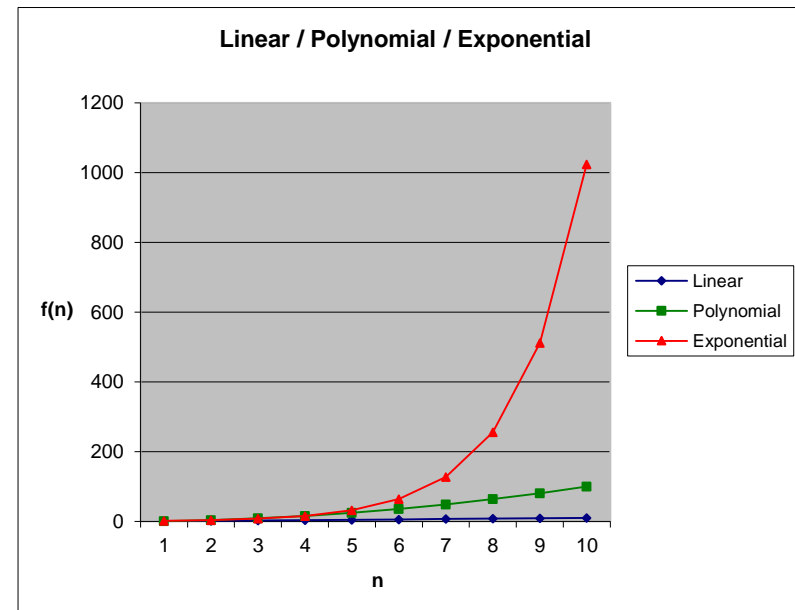
- Natural Language processing
 - Information extraction, semantic parsing, translation, topic models, ...
- Computer vision
 - Object recognition, scene analysis, segmentation, tracking, ...
- Computational biology
 - Pedigree analysis, protein folding and binding, sequence matching, ...
- Networks
 - Webpage link analysis, social networks, communications, citations,
- Robotics
 - Planning & decision making

Complexity of Reasoning Tasks

- Constraint satisfaction
- Counting solutions
- Combinatorial optimization
- Belief updating
- Most probable explanation
- Decision-theoretic planning

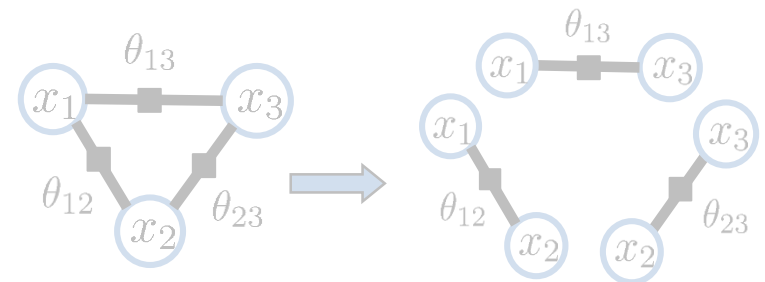
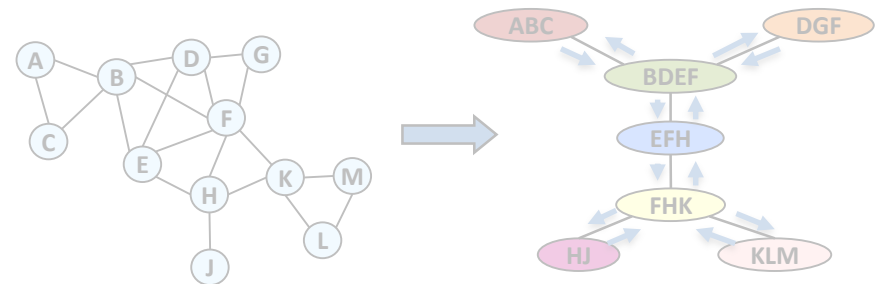
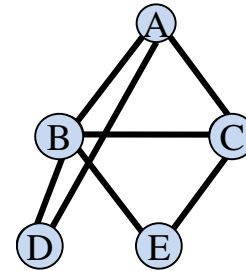
**Reasoning is
computationally hard**

**Complexity is
Time and space(memory)**



RoadMap: Introduction and Inference

- Basics of graphical models
 - Queries
 - Examples, applications, and tasks
 - **Algorithms overview**
- Inference algorithms, exact
 - Bucket elimination for trees
 - Bucket elimination
 - Jointree clustering
 - Elimination orders
- Approximate elimination
 - Decomposition bounds
 - Mini-bucket & weighted mini-bucket
 - Belief propagation
- Summary and Class 2



Types of queries

▶ Max-Inference	$f(\mathbf{x}^*) = \max_{\mathbf{x}} \prod_{\alpha} f_{\alpha}(\mathbf{x}_{\alpha})$
▶ Sum-Inference	$Z = \sum_{\mathbf{x}} \prod_{\alpha} f_{\alpha}(\mathbf{x}_{\alpha})$
▶ Mixed-Inference	$f(\mathbf{x}_M^*) = \max_{\mathbf{x}_M} \sum_{\mathbf{x}_S} \prod_{\alpha} f_{\alpha}(\mathbf{x}_{\alpha})$

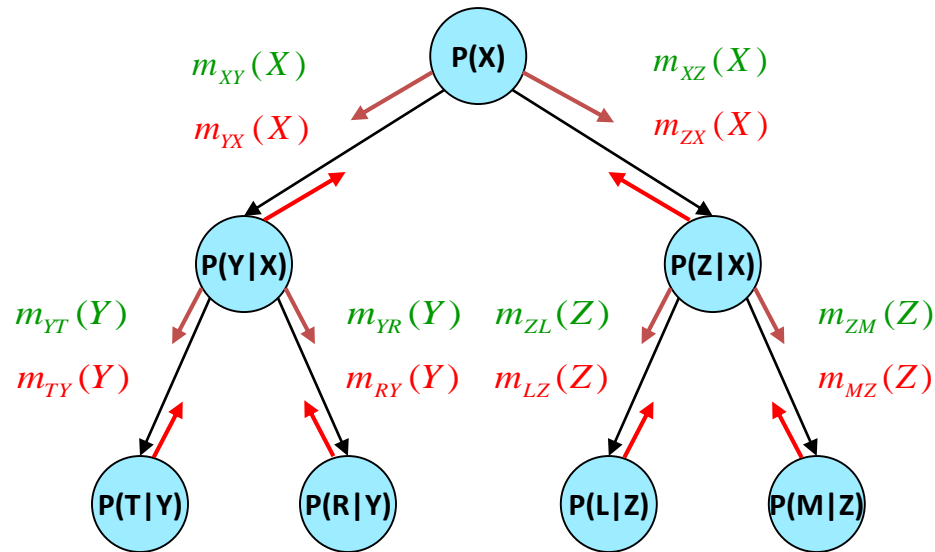


- **NP-hard**: exponentially many terms
- We will focus on **approximation** algorithms
 - **Anytime**: very fast & very approximate ! Slower & more accurate

Tree-solving is easy

**Belief updating
(sum-prod)**

**CSP – consistency
(projection-join)**



MPE (max-prod)

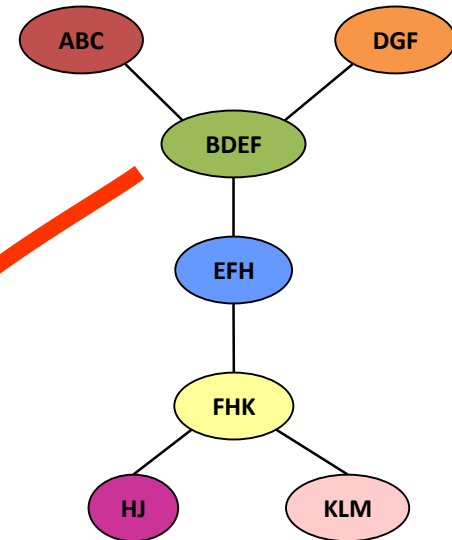
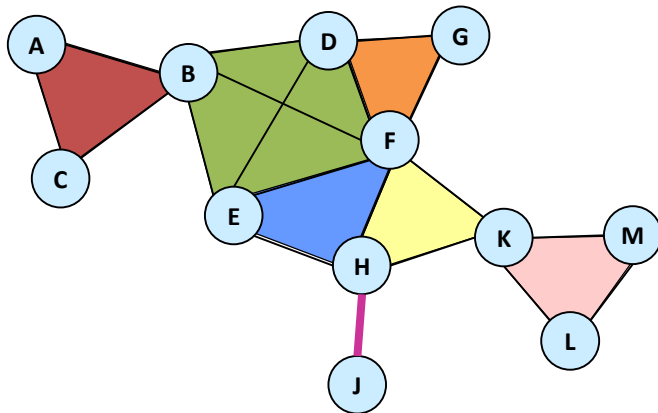
#CSP (sum-prod)

Trees are processed in linear time and memory

Transforming into a Tree

- **By Inference (thinking)**
 - Transform into a single, equivalent tree of sub-problems
- **By Conditioning (guessing)**
 - Transform into many tree-like sub-problems.

Inference and Treewidth



Inference algorithm:

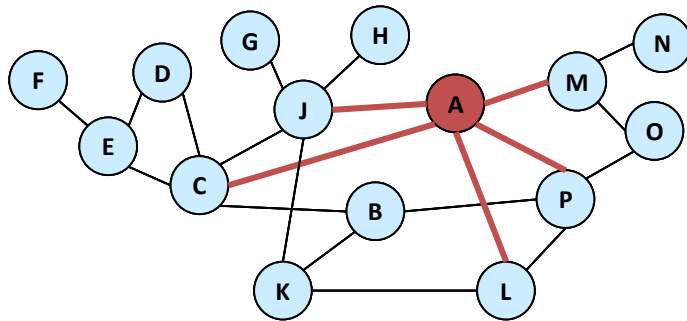
Time: $\exp(\text{tree-width})$

Space: $\exp(\text{tree-width})$

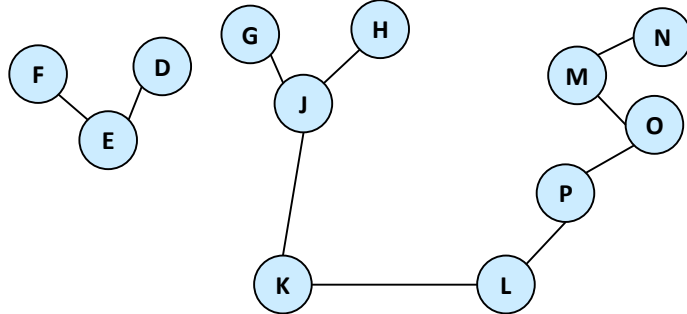
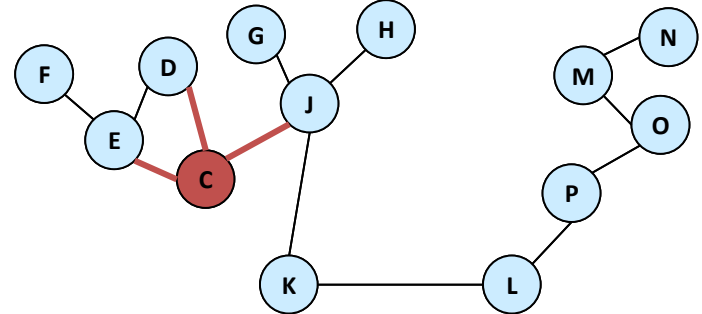
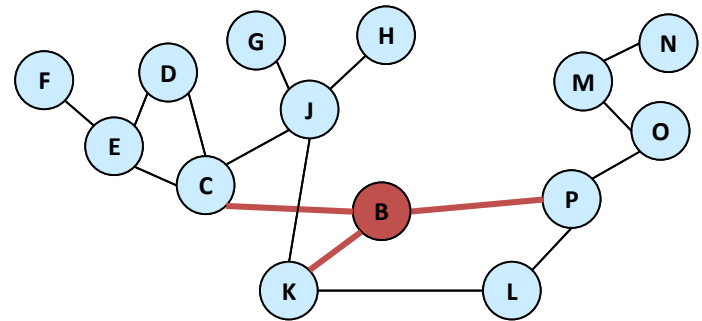
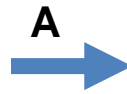
$$\text{treewidth} = 4 - 1 = 3$$

$$\text{treewidth} = (\text{maximum cluster size}) - 1$$

Conditioning and Cycle cutset

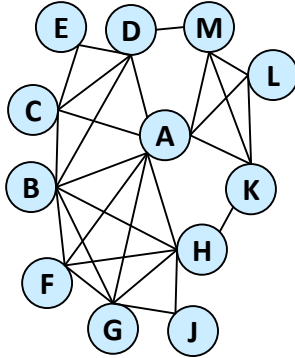


Cycle cutset = {A,B,C}

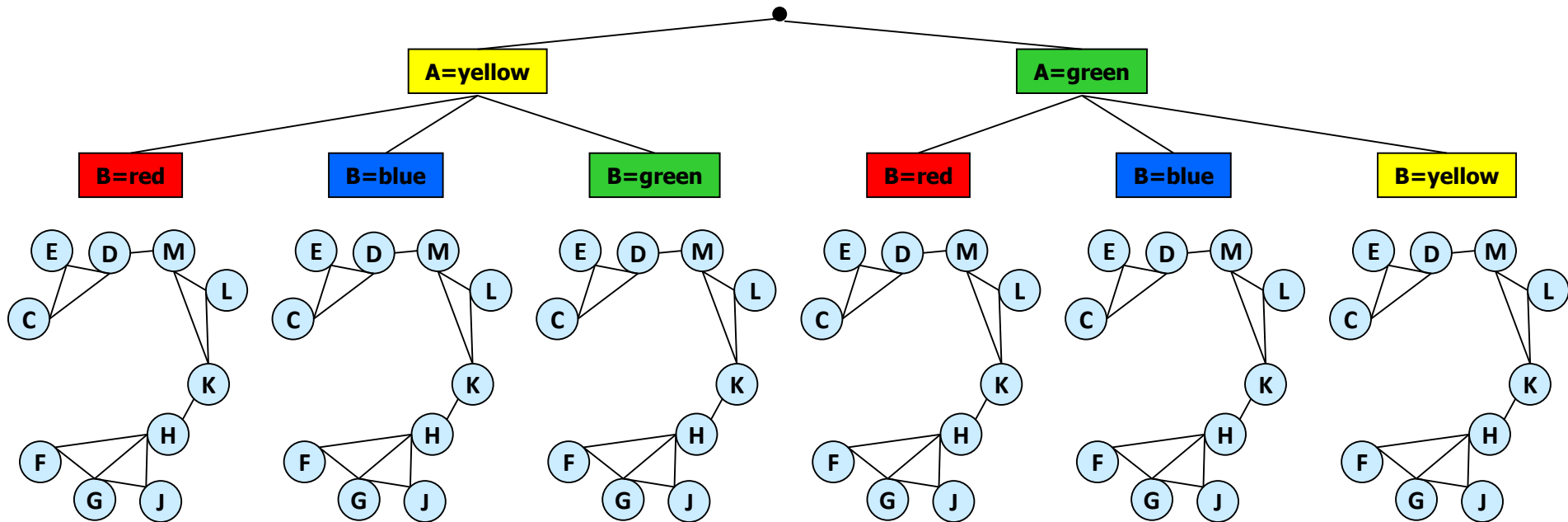


Search over the Cutset

Graph
Coloring
problem



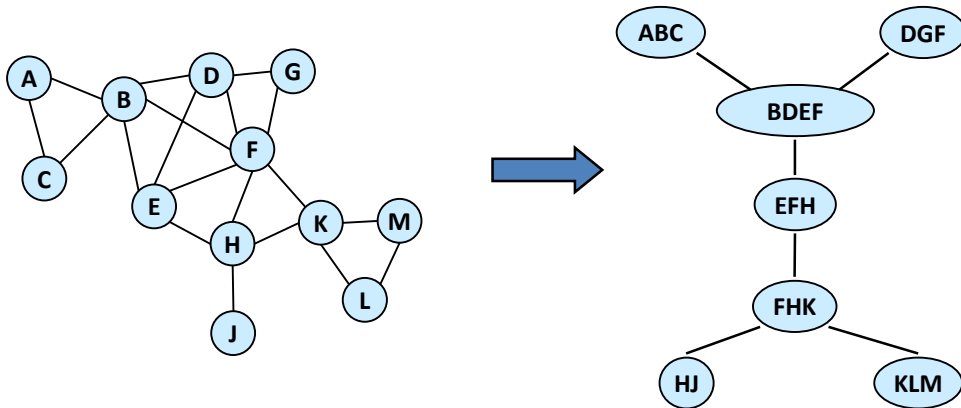
- Inference may require too much memory
- **Condition** on some of the variables



Bird's-eye View of Exact Algorithms

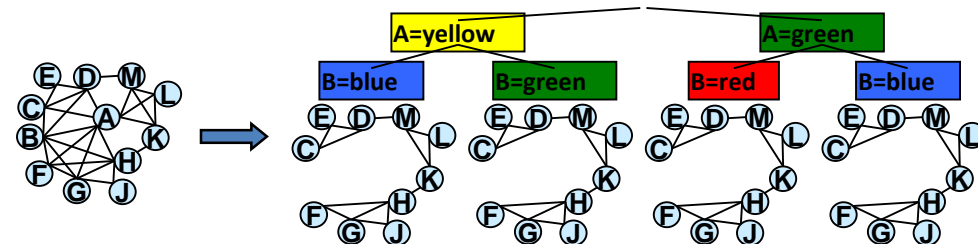
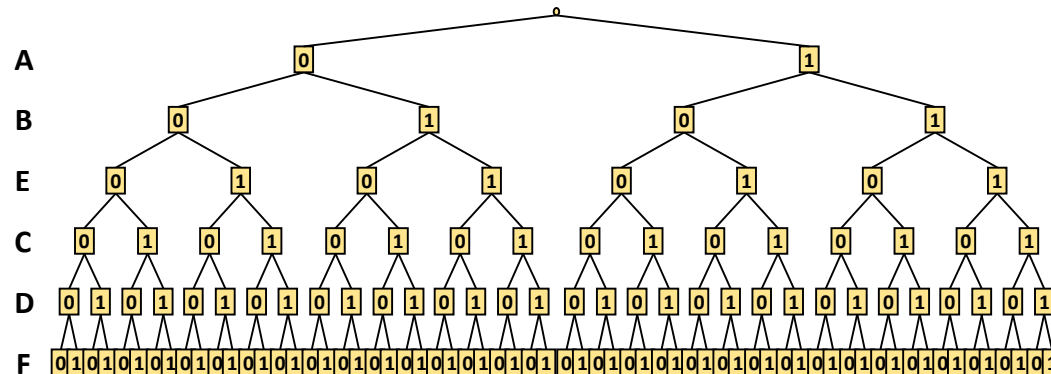
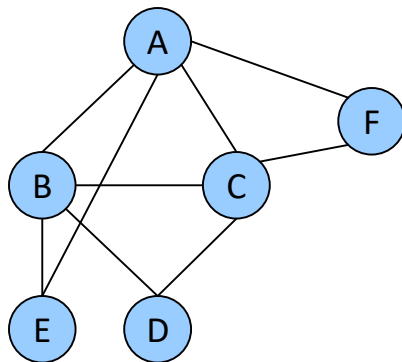
Inference

$\exp(w^*)$ time/space



Search

$\exp(w^*)$ time
 $O(w^*)$ space



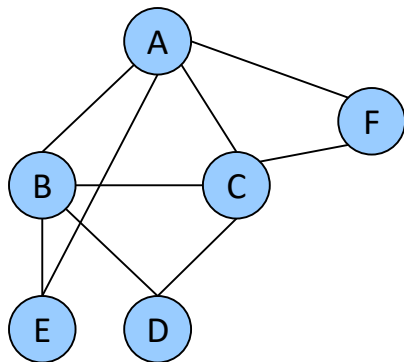
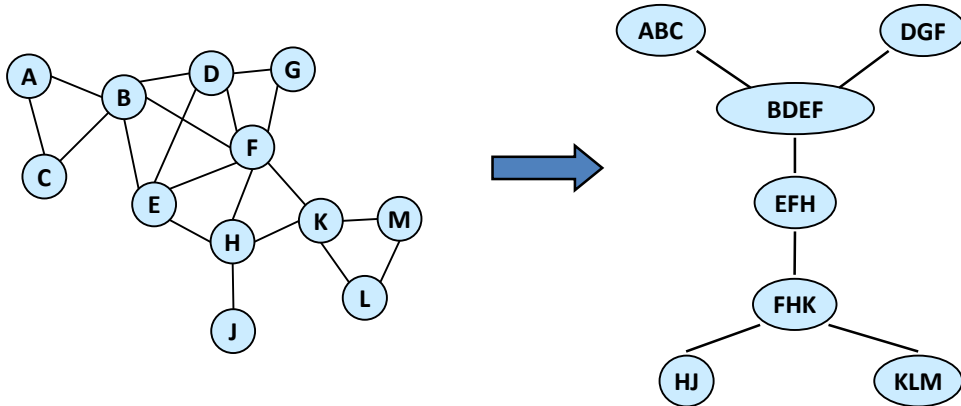
Search+inference:
Space: $\exp(q)$
Time: $\exp(q+c(q))$

q: user
 controlled

Bird's-eye View of Exact Algorithms

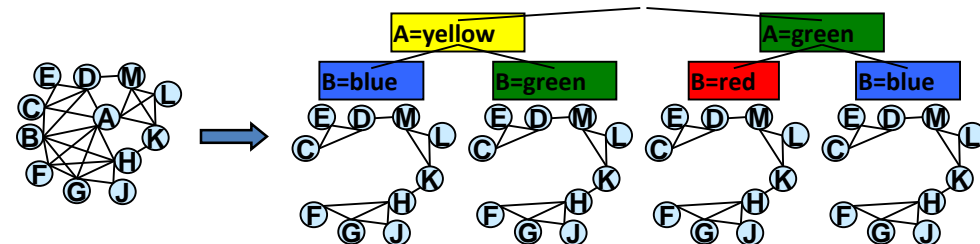
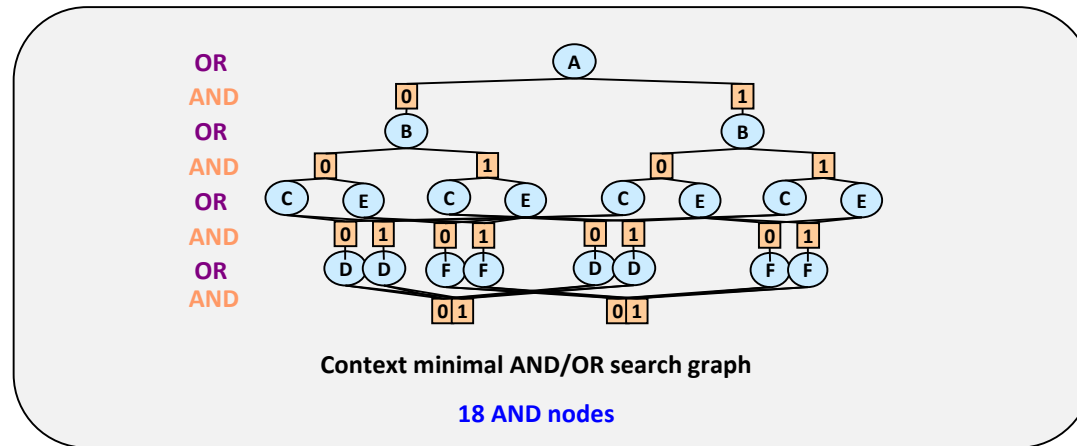
Inference

$\exp(w^*)$ time/space



Search

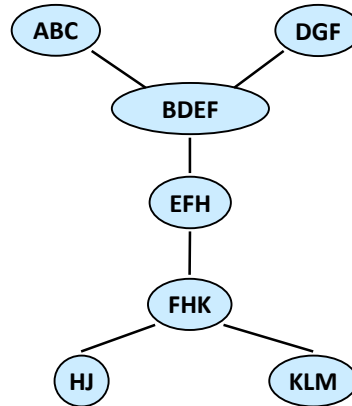
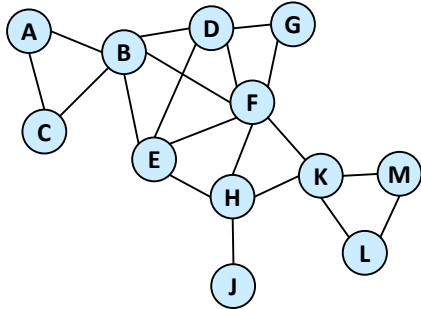
$\exp(w^*)$ time
 $O(w^*)$ space



Search+inference:
Space: $\exp(q)$
Time: $\exp(q+c(q))$

q: user
controlled

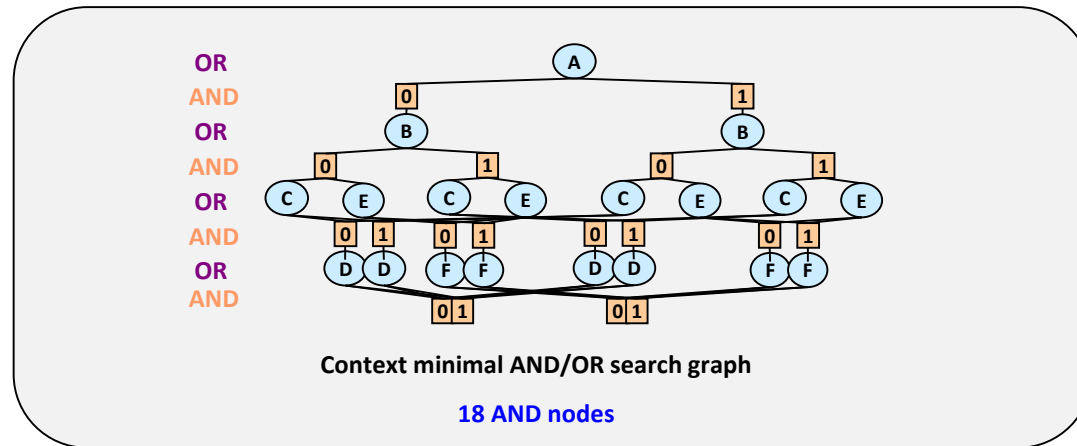
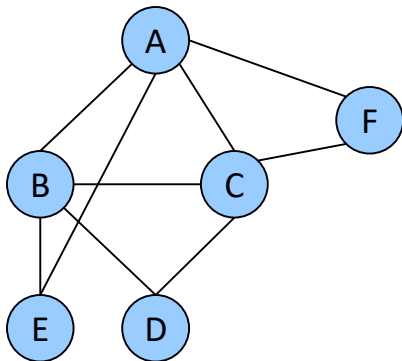
Bird's-eye View of Approximate Algorithms



Inference



Bounded Inference



Search



Sampling

Search + inference:



Sampling + bounded inference

